Session: 2D Semiconductors

(Invited) Transistors based on heterostructures of 2D materials

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Native graphene has a zero energy gap and it is therefore not suitable as a transistor channel material for digital electronics. However, recent advances based on materials engineering have demonstrated "*materials on demand*", with tailored properties. *Vertical heterostructures* of graphene and 2D materials have been proven to be suitable for FETs and hot-electron transistors exhibiting large current modulation.

Inspired by recent progress in the growth of seamless *lateral 2D heterostructures*, lateral heterostructure (LH)-FETs have been proposed, exhibiting extremely promising switching behavior in terms of leakage current, propagation delay, and power-delay product.

We investigate the performance and the scaling perspectives of transistors based on heterostructures of two-dimensional materials against the requirements set by Semiconductory Industry Roadmaps for CMOS (first ITRS and then IRDS). We show that LH-FETs are very promising for high performance logic, down to the 3-5 nm gate length, depending on the types of materials. On the other hand, vertical heterostructure FETs exhibit intrinsic delay times higher by four orders of magnitude, due to large capacitance and poor electrostatics.

We also address some critical aspects related to the modeling of off-plane and in-plane transport in heterostructures of 2D materials.

Monte Carlo study of high field transport in some transition metal di-chalcogenides

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In recent years, there has been a push to find new materials which may have application in the electronics industry. The monolayer compounds came to the forefront when single layers of graphene were isolated [1]. The success of graphene for some applications has led to the investigation of the monolayer transition-metal di-chalcogenides (TMDCs) [2,3,4]. Indeed, field-effect transistors have been created in some of these TMDCs [5]. Of interest in these materials for device applications are specifically the saturated value of the velocity at high electric fields and the possibility of impact ionization within the channel of the device [5,6]. Recently, we have reported the theoretical study of transport in MoS_2 at moderate to high electric fields [7]. Here, we report the studies of transport at higher electric fields in both MoS_2 and WS_2 with the use of the ensemble Monte Carlo technique. These materials are monolayers in which each layer is composed of Mo or W atoms at the center of the layer and S atoms displaced above and below this center. In bulk form, they have an indirect band gap, which becomes direct only in the monolayer limit. The band extrema are located at the K and K' points of the Brillouin zone, so that there are two minima for the conduction band. Subsidiary valleys of the conduction arise from the residual valleys of what was the indirect gap. These valleys, referred to as the T valleys [8], lie midway between Γ and K on the connecting line between these two points. The conduction band mass is approximately $0.45(0.32)m_0$ in the K valleys and $0.57(0.52)\ m_0$ in the subsidiary valley for $MoS_2(WS_2)$. These satellite valleys lie some 200(50) meV above the K valleys. These bands are non-parabolic, and this has to be taken into account for high field transport. We consider impact ionization initiated in both sets of conduction band valleys with a two- dimensional model based upon our

old work [9]. Scattering of carriers in the K valleys, and between them, is dominated by the acoustic phonons and the homopolar and LO optical phonons, which are scattered via the deformation potential interaction. These are the Γ (intravalley) and K (equivalent intervalley via the LO) phonons responsible for scattering in the K valleys. Scattering between the K valleys and the T valleys is via T point LO phonons. Similarly, the scattering between the various T valleys is by these same phonons. The coupling constants for the various phonon modes have been determined from DFT calculations by Kaasbjerg et al. [10], and we use these values in the computation. We include Coulomb scattering from remote ionized impurities connected with the SiO_2 upon which the monolayer is deposited. A nominal density of 0.3–1.0 × 10^{12} cm^{-2}, with a uniform distribution on the surface of the oxide, is assumed. In Fig. 1, the velocity at high fields is plotted for a carrier density of 2 × 10^{12} cm^{-2}. We find that the apparently velocity is weakly dependent upon the carrier density, although it varies more significantly as the impurity density is varied. It is clear that saturation sets in a relatively modest values of the electric field and that there appears to be a slight negative differential conductance (NDC) at higher fields. This effect is not due to intervalley transfer, as most carriers are in the satellite valleys well before the onset of this behavior. It is more likely a result of increased scattering in the two dimensional material and streaming in the distribution function, as we will see below. In Fig. 2, the fraction of carriers that remain in the K and K' valleys is plotted, so that it is clear this is greatly reduced prior to the onset of the NDC. In Fig. 3, the distribution function at two different values of the field are shown for WS_2. At the higher field, the distribution is deviating from a thermal behavior and exhibiting streaming which can contribute to the NDC as the carriers move to higher energies and therefore more scattering in the non-parabolic bands. Finally, in Fig. 4, we plot the observed generation rate for impact ionization as a function of the inverse field. The linear behavior on this plot is a sign of this effect being due to quasi-ballistic carriers, the so-called "lucky electron" model [11].

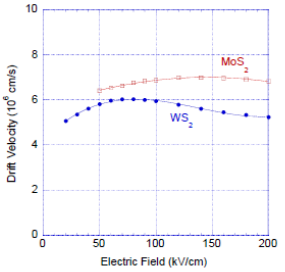

Fig. 1 Velocity as a function of the electric field.

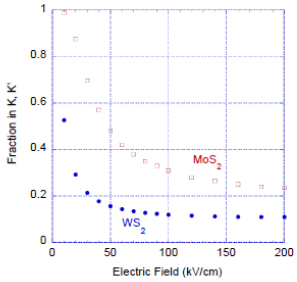

Fig. 2 Fraction of carriers that remain in the K and K' valleys.

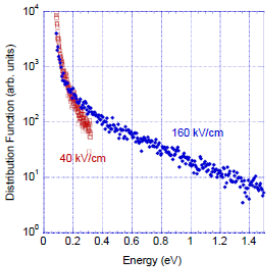

Fig. 3 Distribution function for two fields in WS_2.

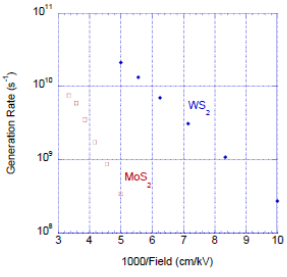

Fig. 4 Impact ionization generation rates as a function of the inverse field.

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Stark effect in the photoluminescence of transition metal dichalcogenide structures

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Transition metal dichalcogenides (TMDs) are promising material candidates for next generation nanodevices due to few-atom device thickness and best imaginable gate control. In contrast to e.g. graphene, TMD offers a finite band gap which makes it suitable for transistors [1]. Van der Waal bonded layers are interesting for thin and flexible photovoltaics [2]. To identify the interlayer coupling, the band structure variation with different layer thicknesses and its gate field dependence is assessed here.

The electronic Hamiltonian and basis functions of density functional theory simulations (GGA with PBE [3] using the VASP software [4]) are used (within the Wannier90 software [5]) to extract an electronic Hamiltonian of a TMD unit cell in MLWF representation. This unit cell Hamiltonian is repeated in the NEMO5 software [6] to generate a real-size device Hamiltonian and solve for electronic densities. For charge self-consistency, the Schrödinger equation is iteratively solved with the Poisson equation in sub-atomic resolution, simplifying the spatial shape of Wannier functions with Gaussian functions (σ =0.6 Å). All assessed structures are close to the experimental setups of Ref. [2] with the same oxide capacitance and gate voltage.

The equivalent oxide thickness is set to be 300nm. The channel consists of one to ten layers of MoS_2 with doping deducted from current measurement. On the gate side, a Dirichlet boundary condition is used to set the gate voltage value. The top side is exposed to vacuum and a Neumann boundary condition of flat band (zero electric field) is applied.

Using the relaxed lattice, MLWF-calculated bandstructures are found to agree with ab-initio calculations for any TMD layer thickness [7]. The conduction band minimum in 2D momentum space is shown in in agreement with Ref.[9] Two inequivalent valleys exist with non-isotropic and layer dependent effective masses (in agreement with Ref.[9]), K and Q valley are the lowest for the conduction while K and Γ highest for the valence band. With increasing layer thickness, the bandedge shifts from K to Q (K and Γ) valley around 2 layer for the conduction(valence) bands as shown in Fig. 2. Fig. 3 compares the bandstructure of a 5-layer thick MoS2 system with and without a finite gate bias applied. Without electric fields, the K-valley is 5-fold degenerate. The finite gate field lifts this degeneracy and reduces the energy separation between K and Q valleys. This indicates the wavefunction localization differs for different valleys and the bandgap is tunable with electric gate fields. This is observed in Fig. 4 with a red shift of the PL spectrum – in good agreement with experimental data.